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Magnetic hysteresis in Ising-like dipole-dipole model

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Abstract

Using zero temperature Monte Carlo simulations we have studied the magnetic hysteresis in a three-dimensional Ising model with nearest neighbor exchange and dipolar interaction. The average magnetization of spins located inside a sphere on a cubic lattice is determined as a function of magnetic field varied periodically. The simulations have justified the appearance of hysteresis and allowed us to have a deeper insight into the series of metastable states developed during this process.

05.50.+q, 05.70.Ln, 75.40.Mg, 75.60.Ej

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I. INTRODUCTION

The description of hysteresis—predominantly for magnetization curves—has been the aim of numerous papers for more than a century now. The early phenomenological model of Lord Rayleigh was the fundamental idea of the well known Preisach-model of ferromagnetic hysteresis, which has been further developed and widely discussed together with other descriptive phenomenological models in a long series of works [1] appearing up till the present days. The physical explanation for the lag of the magnetization component behind the external magnetic field varying along a given line was elaborated by Stoner and Wohlfarth [2] in a simple micromagnetic model for the case of a single-domain particle of uniform magnetization. With the advance of the technics of statistical physics recently great interest seems to be oriented towards the investigation of hysteretic phenomena in realistic multi-particle and/or multi-domain systems. The aim after all would be narrowing the gap between the phenomenological "top-down" and the physical "bottom-up" approaches to the description of hysteresis in general.

In this paper Monte Carlo simulation of a multi-particle Ising system of point-like elementary magnetic dipoles will be presented. The dipoles contained inside a sphere are arranged in a three-dimensional simple cubic lattice, they are parallel or antiparallel to the z-axis of the Cartesian system and interact by the nearest neighbour exchange as well as the long-range dipole-dipole couplings.

It will be shown that this model exhibits magnetic hysteresis if the external magnetic field is varied periodically. The present approach allows us to visualize and analyse the evolution of spin configurations.

II. THE MODEL

We consider a three-dimensional Ising model with spins located on the points of a simple cubic lattice ($\mathbf{r} = (x, y, z)$; x, y, and z are integers) within a sphere of radius R ($r^2 = x^2 + y^2 + z^2 < R^2$). Dimensionless quantities will be used throughout the paper. Namely, the length will be measured in terms of lattice constant a, the dipole moments in terms of the unique dipole moment μ, the external magnetic field h will be expressed in units of μ/a^3 and the energy per spins in terms of μ^2/a^3. In this case the Hamiltonian is given by

$$H = -J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \sigma(\mathbf{r})\sigma(\mathbf{r}') - h \sum_{\mathbf{r}} \sigma(\mathbf{r}) + \frac{1}{2} \sum_{\substack{\mathbf{r},\mathbf{r}' \\ \mathbf{r} \neq \mathbf{r}'}} V(\mathbf{r} - \mathbf{r}')\sigma(\mathbf{r})\sigma(\mathbf{r}') \tag{1}$$

where $\sigma(\mathbf{r}) = 1$ and -1 for up and down spins. In the first term the sum is over the nearest-neighbor pairs and J denotes the strength of the usual exchange interaction measured in the above mentioned energy unit. The second term describes the effect of the external magnetic field h. The dipole-dipole interaction between two spins having only z component is defined as

$$V(\mathbf{r}) = \frac{r^2 - 3z^2}{r^5} \quad . \tag{2}$$

Notice that this dipole-dipole interaction provides ferromagnetic coupling along the z axis and the coupling becomes antiferromagnetic in the $x - y$ plane. Furthermore, the average

value of the field of a given dipole over the points located at a prescribed distance vanishes due to the cubic symmetry. Conversely, up (or down) spins on a “spherical shell” produces zero magnetic field at the central lattice point. This is the reason why the resultant magnetic field is zero at the center of a spherical sample if all the spins point to up (or down). [3–6] At a given site $\mathbf{r}$ the magnetic field produced by the remaining dipoles is given as

$$h_d(\mathbf{r}) = -\sum_{\substack{\mathbf{r}' \\ \mathbf{r}' \neq \mathbf{r}}} V(\mathbf{r}-\mathbf{r}')\sigma(\mathbf{r}') \ . \tag{3}$$

Our analysis is restricted to spherical systems because here the early theories predicts zero field inside the ferromagnetic sphere. [3–6] More precisely, Cohen and Keffer [6] have shown that the contribution of point-like dipoles to the local field may differ from zero in the close vicinity of the surface. We have numerically studied the local field because this phenomenon plays crucial role in the magnetic hysteresis as will be described in the next section.

In the ferromagnetic state the average $h_d(\mathbf{r})$ (energy per sites) due to dipolar interactions is zero [5] independently of the system size. In this case the local field satisfies the conditions of reflection ($h_d(x,y,z) = h_d(\pm x, \pm y, \pm z)$) and rotation ($h_d(x,y,z) = h_d(-y,x,z)$) symmetries. The numerical results (see Fig. 1) demonstrate clearly that inside our sphere $h_d(\mathbf{r}) \approx 0$ in agreement with the predictions of analytical calculations [3–6]. At the same time large variations are indicated on the outer shells. For $\sigma(\mathbf{r}) = +1$ the highest values of h_d appear along the periphery of the top and bottom layers. Along the (1,1,1) directions the local field vanishes (see the open circles in Fig. 1). The lowest field values are found at the 8 sites symmetrically equivalent to (15,0,3) if $R = 15.33$.

The probability distribution of the lattice points as a function of h_d exhibits a sharp peak around $h_d = 0$, and its maximum value increases with R. In a cube-shaped sample such calculation yields a significantly different (wide) probability distribution which causes drastic changes in the hysteresis too.

The dipolar energy of ordered spin configurations was determined previously in infinite systems of cubic symmetry. Using the Ewald method Luttinger and Tisza [5] evaluated the energy per sites for all the (periodic) ordered structures characterized by a spin configuration within the $2 \times 2 \times 2$ unit cell. In the energetically favoured states the up (or down) spins form vertical columns as expected. For $h = 0$ and $J = 0$ the spin configuration of lowest energy is a twofold degenerated chess-board-like antiferromagnetic arrangement in the $x-y$ plane of ferromagnetic columns along the z direction, that is $\sigma(\mathbf{r}) = 1$ (-1) if $x+y$ is odd (even). In this columnar antiferromagnetic (CAF) structure the energy per sites is given as [5]

$$E_{CAF} = -2.676 + J \ . \tag{4}$$

Furthermore, for the fourfold degenerated layered antiferromagnetic (LAF) spin configuration, where $\sigma(\mathbf{r}) = 1$ (-1) if x (or y) is odd (even), the energy per sites is

$$E_{LAF} = -2.422 - J \ . \tag{5}$$

It is obvious from Eqs. (4) and (5) that the CAF state is preferred to LAF if the ferromagnetic coupling $J < 0.127$. In our spherical model numerical calculations are performed to check the finite size effects choosing $R = 10.25$, 12.25 and 15.33. For both the above mentioned spin

configurations it is found that finite size corrections are proportional to $1/R$. The numerical technique has allowed us to study periodic antiferromagnetic structures different from those studied by Luttinger and Tisza [5]. These calculations indicate that double or multilayer structures (similar to LAF) become stable for sufficiently strong ferromagnetic coupling and the preferred layer width increases with J. These indications, however, should be considered as preliminary results because more systematic analyses are required to investigate the effect of (anti)ferromagnetic coupling on the spin configurations in the ground state, the size effects, *etc.* Henceforth, we will concentrate on the model with $J = 0$. In this case the slow cooling Monte Carlo technique has confirmed that the twofold degenerated ground state is equivalent to the CAF spin configuration in zero external field ($h = 0$).

III. SIMULATION OF HYSTERESIS

A series of zero temperature Monte Carlo simulations has been performed to study hyteresis phenomena in the model described above. In these simulations the system is started from a random spin configuration. For an elementary process a randomly chosen spin is flipped if $(h_d(\mathbf{r}) + h)\sigma(\mathbf{r}) < 0$, otherwise the spin value remains unchanged. This process is repeated until all the spin signs become equivalent to the sign of the local magnetic field. Then the external magnetic field (h) is increased (decreased) by Δh and repeating the above mentioned spin flipp processes the system is allowed to relax toward a new local energy minimum. In such a way the external field is varied periodically with an amplitude of 10. During this procedure we monitored the magnetization defined as

$$m = \frac{1}{N} \sum_{\mathbf{r}} \sigma(\mathbf{r}) \tag{6}$$

where N is the number of spins inside the sphere. These simulations have clearly indicated the appearance of the usual magnetic hysteresis. A typical result obtained for $J = 0$, $R = 15.33$ and $|\Delta h| = 0.1$ is shown in Fig. 2. To check the size effect the simulations have been carried out for different sizes ($R = 10.25$ and 12.25). The comparisons have indicated that the size effect is comparable to the uncertianty of data observed between subsequent cycles (see Fig. 2). In other words, the above mentioned system size containing 15 203 spins is sufficiently large to study the hysteresis adequately in this model. Unfortunately, for larger sizes the simulation becomes very time-consuming because the computational time is proportional to R^6. The choice of $|\Delta h| = 0.1$ is also motivated by the minimization of run time. Further decrease of Δh does not modify the plotted curves significantly.

Figure 2 indicates the presence of avalanches when varying the magnetic field. Similar phenomena were observed in experiments by Barkhausen [7] and also in the random field Ising models [8]. Recently different approaches are used to study the avalanches as well as its relation to the hysteresis. [9,10] In the present model the appearence of avalanches is a consequence of dipole-dipole interaction.

By varying the magnetic field several spins of the actual configuration becomes preferred to flip into the opposite state. Reversing a randomly chosen spin the local field $h_d(\mathbf{r})$ will be modified in all sites of the system. Due to the dipole-dipole interaction the neighboring spins in the same column are favoured to change direction too. This effect drives the avalanche of spin flips in a given column. During the simulations the spin flips are observed in several

columns simultaneously. This process leads predominantly to such configurations where complete spin columns have been reversed as demonstrated in Fig. 3.

Figure 3 shows six spin configurations appeared at different magnetic fields during a half-cycle when decreasing h from 10. In order to visualize a more complete 3D picture on the spin configurations parts of the horizontal ($z = 0$) and vertical ($x = 0$) cross sections are displayed by removing a quarter of spins from the sphere. In this figure the small black spheres with white border and the white spheres with black border indicate up and down spins.

Decreasing the magnetic field the initial saturated state ($m = 1$) remains unchanged until $h = 2.253$ whose value depends slightly on R. For the given size the spins which can be the first to flip are positioned at one of the 8 sites equivalent to $(15, 0, 3)$. Consequently, the spins in the corresponding four columns can flip simultaneously, because the short columns are too far to affect each other significantly. The result is well recognizable for a possible subsequent configuration plotted in picture a. Notice that here the mentioned symmetries are no longer valid due to a branching process described as follows. Immediately after the decrease of h some of the spins become reversible. One of them is chosen randomly to flip. This elementary process fastened by the above mentioned columnar spin flip avalanche can actually prevent the flips at the "rival spins". Thus the order of consecutive steps during the formation of the subsequent columnar structures (see Fig. 3) is occasional. This phenomenon causes the hysteresis curves to be unreproducable for finite sizes as demonstrated in Fig. 2.

Configuration c in Fig. 3 represents a typical state with a remanent magnetization when reaching $h = 0$. The magnetization vanishes at $h \simeq -1$. Here, the appearence of domains with CAF and LAF structures are striking (see configuration d). The CAF state dominates the vicinity of the z axis. The positions of the LAF domains are initialized by the first columnar spin flips after saturation. These domains remains recognizable in a wide range of the magnetization process as indicated by the configuration e obtained for $h = -2$. Further decrease of h will destroy these ordered regions leaving the spins unchanged only in a few columns positioned randomly (configuration f for $h = -6$). Notice that this configuration differs significantly from the initial ones (compare to a). Finally all the spins point to downward if the magnetic field becomes less than -6.2.

When studying a more complete series of spin configurations one can easily recognize that the back spin flips appears rarely upon a half-cycle. According to our numerical investigations the number of back spin flips is less than 1% of the total number of spins. During the simulations we have also recorded the number of non-uniform columns which is found to be zero in the initial and final stages of demagnetizing processes. This number can occasionally differ from zero and its rate remains below 1%.

The low number of back flips explains the phenomena observed when we have articially prevented the free spin flips. In this case the above described dynamics is modified by assuming a hysteretic behavior for the individual spins. Namely, the spin flips may occur for the randomly chosen sites only if the driving force exceeds a threshold value ($f_t \geq 0$). Evidently, for $f_t = 0$ this modification leaves the above results unchanged. In agreement with the expectation the hysteresis loop becomes wider for pozitive f_t. More precisely, the "sides" of the loops are shifted outward without causing any observable changes in the slopes. This means that the main features of the subsequent spin configurations are similar to those described above (see Fig. 3) and the columnar spin flips are delayed within the

cycles. However, the number of back flips (during the half-cycle) decreases with f_t. For example, only a few back flips can be observed for $R = 15.33$ and $f_t = 1$ and this elementary process vanishes practically if $f_t > 2$.

Finally we have investigated the effect of ferromagnetic coupling ($J > 0$) on the hysteresis. For this purpose the hysteresis curves are recorded for different J values as shown in Fig. 4. In this case the simulations are started from the ferromagnetic state ($h = 10$). We have observed that the extension of avalanches (as well as the uncertainty of the magnetization process for the subsequent cycles) increases with J. Figure 4 demonstrates that these phenomena are accompaned with the increase of average slope along the "side" of loops and the broadening of the hysteresis loop. These observations are related to formation of larger and larger ferromagnetic domains as well as the more and more massive avalanches when increasing the ferromagnetic coupling.

One can observe that the initial steps of the demagnetization process is slightly modified by the nearest-neighbor couplings because the first spin flips appear on the surface at low latitudes where $h_d(\mathbf{r})$ has low (negative) values. This is the region where the ferromagnetic force is weak because of the low number (three or four) of neighboring spins, therefore it is not able to prevent the spin flips driven by the local field $h + h_d(\mathbf{r})$. Further systematic analysis is required to study what happens when the typical ferromagnetic domain sizes become larger than R.

IV. CONCLUSIONS

Numerical simulations have been performed to investigate the hysteresis phenomena in a three-dimensional Ising model involving both the nearest neighbor exchange and the long range dipolar interactions. For simplicity the spins are located on a cubic lattice within a sphere. This shape provides zero local field $h_d(\mathbf{r})$ inside the sphere for a ferromagnetic state. The large deviations of $h_d(\mathbf{r})$ at the surface are found to play crucial role at the beginning of demagnetization processes started from a saturated state. Using zero temperature Monte Carlo simulations the magnetization process is investigated under an alternating external magnetic field with an amplitude providing complete saturations.

During this process we have observed avalanches and branching points leading to a large variation of paths along which the system can evolve. The avalanches consist of spin flips constrained into a few columns. As a result, after having varied the magnetic field the new stationary (metastable) states built up dominantly from columns with uniform spins. This feature decreases drastically the number of possible metastable state (characterizing the hysteretic behaviour) in comparison to the total number of configurations. Our simulations have justified that the number of back flips is negligible within the half-cycles of magnetization process.

We think that the present model seems to be a good candidate for exploring relationship between a microscopic description and the phenomenological (e.g. Preisach model) approaches of hysteresis. For this purpose, however, we need more detailed information about the internal hysteresis loops, the effects of shape and exchange constant, the local field distribution, etc. Fortunately, the model simulations give us a wide scale of opportunity to have a deeper understanding.

ACKNOWLEDGMENTS

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FIGURES

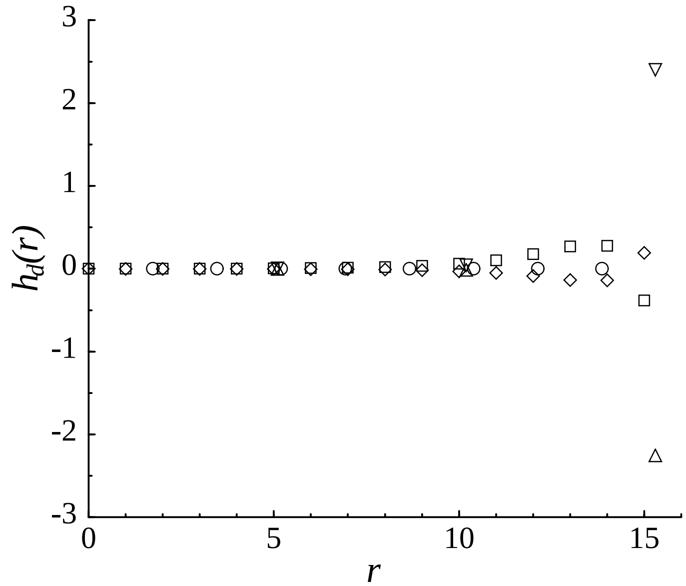

FIG. 1. Radial dependence of the local magnetic field if $m = 1$ and $R = 15.33$ for choosing different directions: (1,0,0) diamonds, (0,0,1) open squares, (1,1,1) open circles, (5,0,1) $\triangle$ and (1,0,5) $\bigtriangledown$.

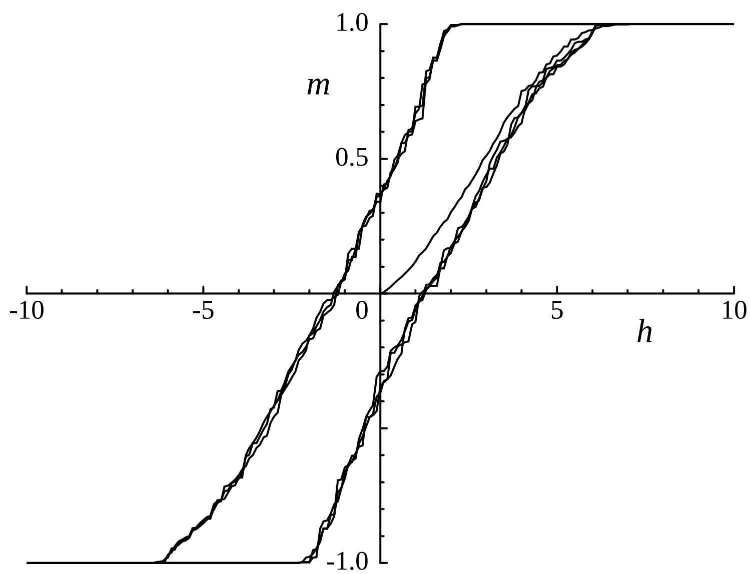

FIG. 2. Magnetic hysteresis for $J = 0$ and $R = 15.33$.

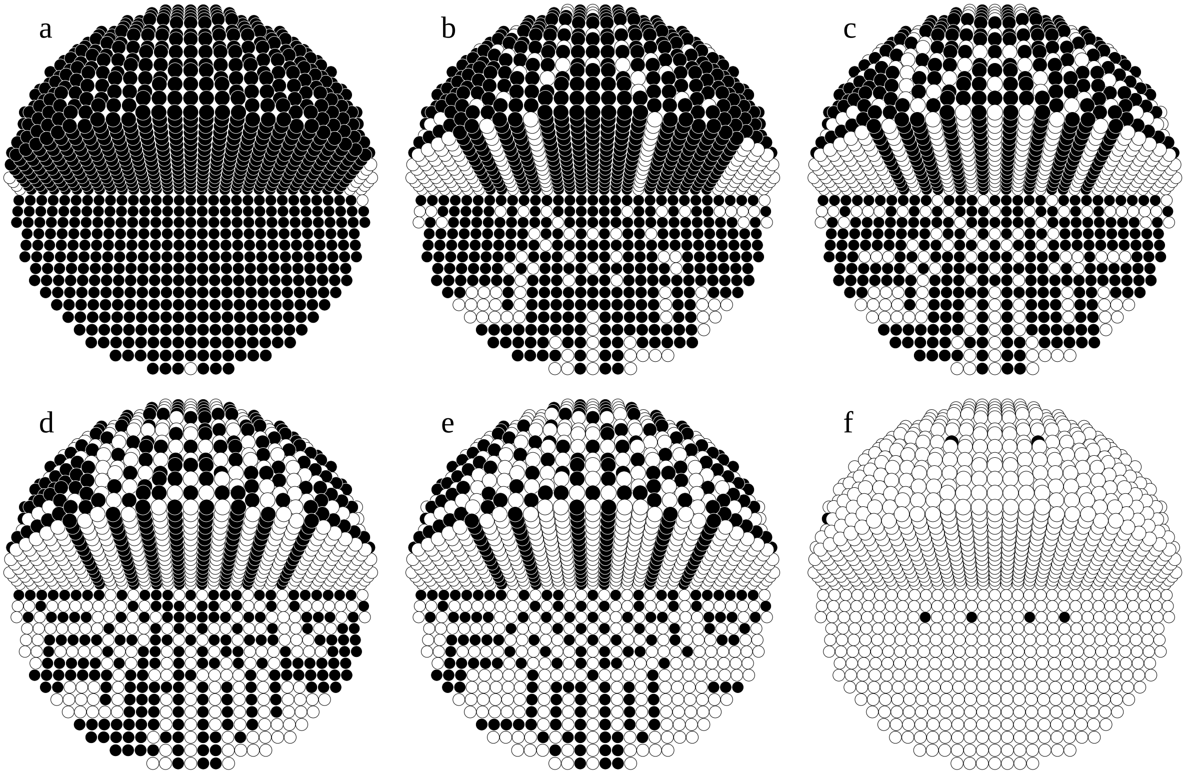

FIG. 3. Spin configurations when decreasing the magnetic field from $h = 10$ to 2 (a); 1.7 (b); 0 (c); -1 (d); -4 (e) and -6 (f). Black and white spheres indicate up and down spins.

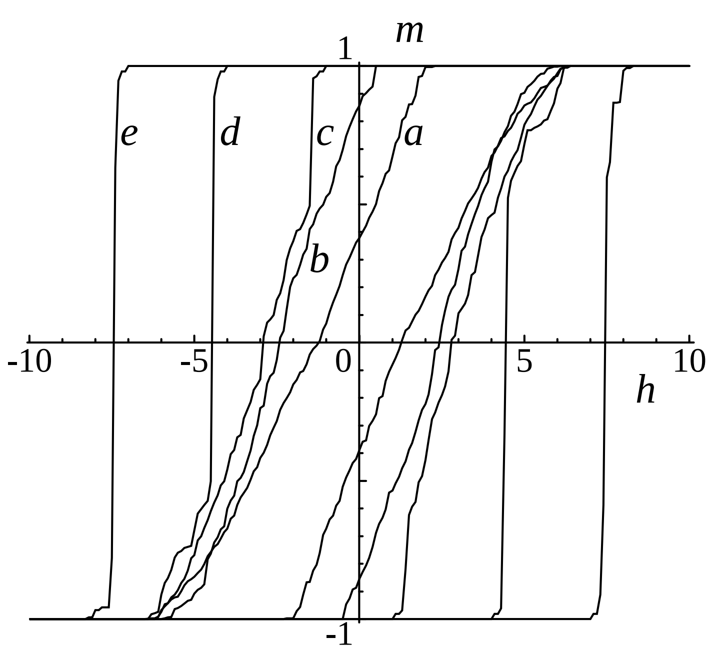

FIG. 4. Magnetic hysteresis curves for different exhange constants: $J = 0$ (a), 0.5 (b), 1 (c), 2 (d) and 3 (e) for $R = 15.33$. The curves are averaged over 10 cycles.